2.4 Modification to Capillary Pressure Functions

Modified versions of the Brooks-Corey and van Genuchten models [*Luckner et al.*, 1989] were implemented. In order to prevent the capillary pressure from decreasing towards negative infinity as the effective saturation approaches zero, a linear function is used for saturations S_l below a certain value $(S_{lr} + \varepsilon)$, where ε is a small number. The slope of the linear extrapolation is identical with the slope of the capillary pressure curve at $S_l = S_{lr} + \varepsilon$. Alternatively, the capillary pressure is prevented from becoming more negative than $-p_{c,\max}$.

The correct implementation is checked by visual inspection of the capillary pressure curves near residual saturation. Capillary pressure vs. saturation data in the range $0 \le S_l \le 1$ are written to a separate file for plotting when ITOUGH2 command `>>> CHARACTERISTIC` is given. The plot file *vvi_ch.tec* was created using the following command line:

```
itough2 -v 3.2 vvi vv 3 &
```

2.4.1 Modification to Brooks-Corey Capillary Pressure Function

The modified Brooks-Corey model is invoked by setting both `IRP` and `ICP` to 10. The model is described by the following set of equations (the input parameters are listed in Table 2.4.1.1):

$$S_{ec} = \frac{S_l - S_{lrc}}{1 - S_{lrc}} \tag{2.4.1.1a}$$

$$S_{ek} = \frac{S_l - S_{lrk}}{1 - S_{lrk} - S_{gr}} \tag{2.4.1.1b}$$

$$p_c = -p_e \left(S_{ec}\right)^{-1/\lambda} \qquad \text{for} \quad S_l \ge (S_{lrc} + \varepsilon) \tag{2.4.1.2a}$$

$$p_c = -p_e \left(\frac{\varepsilon}{1 - S_{lrc}}\right)^{-1/\lambda} - \frac{p_e}{\lambda}\left(\frac{\varepsilon}{1 - S_{lrc}}\right)^{-\frac{1-\lambda}{\lambda}} \left(S_l - S_{lrc} - \varepsilon\right) \qquad \text{for} \quad S_l < (S_{lrc} + \varepsilon) \tag{2.4.1.2b}$$

$$p_c \ge -p_{c,\max} \tag{2.4.1.3}$$

$$k_{rl} = S_{ek}^{\frac{2-3\lambda}{\lambda}} \tag{2.4.1.4a}$$

$$k_{rg} = \left(1 - S_{ek}\right)^2 \left(1 - S_{ek}^{\frac{2+\lambda}{\lambda}}\right) \tag{2.4.1.4b}$$

$$k_{rg} = 1 - k_{rl} \tag{2.4.1.4c}$$

Table 2.4.1.1. Input Parameters for Modified Brooks-Corey Model

Parameter	Variable	Description
IRP	10	select Brooks-Corey relative permeability model
RP(1)	S_{lrk}	residual liquid saturation for relative permeability functions
RP(2)	S_{gr}	residual gas saturation
RP(3)	(flag)	if zero, use (2.4.1.4b), otherwise (2.4.1.4c)
ICP	10	select Brooks-Corey capillary pressure model
CP(1)	λ	pore size distribution index
CP(2)	p_e	gas entry pressure [Pa]
CP(3)	ε or	if CP(3) = 0 then $p_{c,\max} = 10^{50}$, $\varepsilon = -1$
	$p_{c,\max}$	if 0 < CP(3) < 1 use linear model (2.4.1.2b) for $S_l < S_{lr} + \varepsilon$
		if CP(3) ≥ 1, then $p_{c,\max}$ = CP(3), $\varepsilon = -1$
CP(6)	S_{lrc}	if zero, then $S_{lrc} = S_{lrk}$

Figure 2.4.1.1 shows two modified Brooks-Corey capillary pressure functions. The first one, shown by the solid line, was produced with $CP(3) = p_{c,\max} = 7000$, limiting the capillarity to values larger than $p_c = -7000$ Pa. The second curve, shown by the broken line, was produced with $CP(3) = \varepsilon = 0.1$, leading to a linear decrease in capillary pressure for $S_l < S_{lrc} + \varepsilon$, tangential to the standard Brooks-Corey curve at $S_l = S_{lrc} + \varepsilon$.

The curves shown in Figure 2.4.1.1 reflect the intended behavior, fulfilling Requirement 4.1.

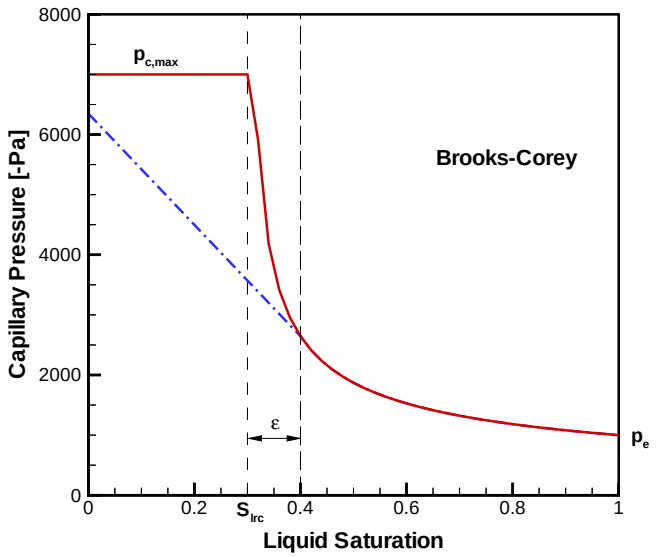

Figure 2.4.1.1. Modified Brooks-Corey capillary pressure curves.

2.4.2 Modification to van Genuchten Capillary Pressure Function

The modified van Genuchten model is invoked by setting both `IRP` and `ICP` to 11. The model is described by the following set of equations (the input parameters are described in Table 2.4.2.1):

$$S_{ec} = \frac{S_l - S_{lrc}}{1 - S_{lrc}} \tag{2.4.2.1a}$$

$$S_{ek} = \frac{S_l - S_{lrk}}{1 - S_{lrk} - S_{gr}} \tag{2.4.2.1b}$$

$$p_c = -\frac{1}{\alpha}\left[\left(S_{ec}\right)^{-1/m} - 1\right]^{1/n} \quad \text{for} \quad S_l \geq (S_{lrc} + \varepsilon) \tag{2.4.2.2a}$$

linear model with continuous slope at $S_l = S_{lrc} + \varepsilon$ for $S_l < (S_{lrc} + \varepsilon)$ (2.4.2.2b)

$$p_c \geq -p_{c,\max} \tag{2.4.2.3}$$

$$k_{rl} = S_{ek}^{1/2}\left[1 - \left(1 - S_{ek}^{1/m}\right)^m\right]^2 \tag{2.4.2.4a}$$

$$k_{rg} = \left(1 - S_{ek}\right)^{1/3}\left[1 - S_{ek}^{1/m}\right]^{2m} \tag{2.4.2.4b}$$

$$k_{rg} = 1 - k_{rl} \tag{2.4.2.4c}$$

Table 2.4.2.1. Input Parameters for Modified van Genuchten Model

Parameter	Variable	Description
`IRP`	11	select van Genuchten relative permeability model
`RP(1)`	S_{lrk}	residual liquid saturation for rel. perm. functions
`RP(2)`	S_{gr}	residual gas saturation
`RP(3)`	(flag)	if zero, use (2.4.2.4b), if non-zero, use (2.4.2.4c)
`ICP`	11	select van Genuchten capillary pressure model
`CP(1)`	n	analogous to pore size distribution index
`CP(2)`	$1/\alpha$	analogous to gas entry pressure [Pa]
`CP(3)`	ε or	if `CP(3)` = 0 then $p_{c,\max} = 10^{50}$, $\varepsilon = -1$
	$p_{c,\max}$	if 0 < `CP(3)` < 1 use linear model (2.4.2.2b) for $S_l < S_{lr} + \varepsilon$
		if `CP(3)` ≥ 1, then $p_{c,\max}$ = `CP(3)`, $\varepsilon = -1$
`CP(4)`	m	if zero then $m = 1 - 1/n$
`CP(6)`	S_{lrc}	if zero, then $S_{lrc} = S_{lrk}$

Figure 2.4.2.1 shows two modified van Genuchten capillary pressure functions. The first one, shown by the solid line, was produced with $CP(3) = p_{c,\max} = 7000$, limiting the capillarity to values larger than $p_c = -7000$ Pa. The second curve, shown by the broken line, was produced with $CP(3) = \varepsilon = 0.1$, leading to a linear decrease in capillary pressure for $S_l < S_{lrc} + \varepsilon$, tangential to the standard van Genuchten curve at $S_l = S_{lrc} + \varepsilon$.

The curves shown in Figure 2.4.2.1 reflect the intended behavior, fulfilling Requirement 4.2.

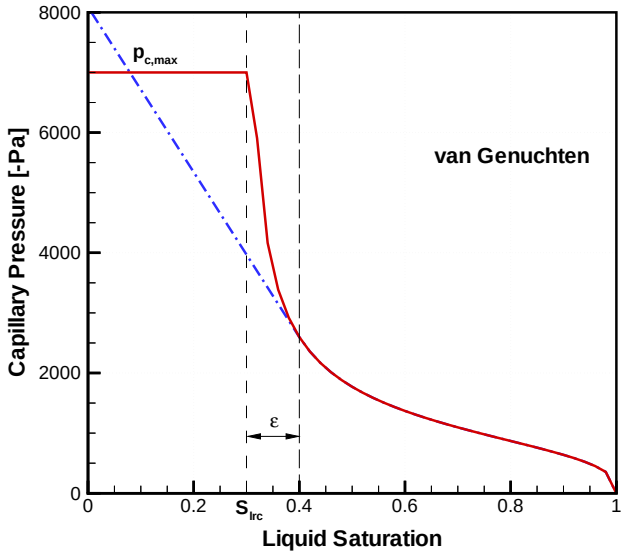

Figure 2.4.2.1. Modified van Genuchten capillary pressure curves.

2.5 New Observation Types

ITOUGH2 estimates TOUGH2 input parameters based on observations for which a corresponding TOUGH2 output variable is calculated. Two new observation types were added, i.e., new output variables are extracted from TOUGH2 and made available for comparison with observed data. In ITOUGH2, the observation type is specified by second-level commands in block `> OBSERVATION`. The first new observation type is selected by command `>> SECONDARY`, extracting the secondary parameters of the specified gridblock. The secondary parameters are the phase-specific fluid properties shown in Table 2.5.1 (see also Figure 2 in *Pruess* [1991]).

Table 2.5.1. Secondary Parameters

Index	Parameter
1	Saturation
2	Relative permeability
3	Dynamic viscosity
4	Density
5	Specific enthalpy
6	Capillary Pressure
NB+k	Mass fraction of Component k

The second new observation type is selected by command `>> HEAT FLOW`, extracting the heat flux of the specified connection.

The correct implementation of the new observation types is checked by comparing the values printed to the TOUGH2 output files with those reported as "computed" in the residual analysis of the ITOUGH2 output file. If they are identical, ITOUGH2 correctly extracted the selected values from the TOUGH2 output arrays.

File *vvi* shown in Figure 2.5.1 was used in combination with the TOUGH2 input file *vv* (see Figure 2.3.1) to generate the requested output. Note that MOP(5) is set to 8 in file *vv* to produce printout of all secondary parameters.

The following command was used:

```
itough2 -v 3.2 vvi vv 3 &
```

The output of this run is also used for testing Requirement 6.

```
> PARAMETERS

--- the following block tests new handling of porosity values,
    i.e., porosity given in block INCON (0.5) will be overwritten by
    initial guess (0.6) for elements with rock type BC___ (ELM 2)

  >> POROSITY
     >>> MATERIAL: BC___
         >>>> VALUE
         >>>> GUESS: 0.6
         <<<<
     <<<
  <<

> OBSERVATION

  >> TIME: 1
     1.0

--- The following blocks test the new observation type SECONDARY

  >> SECONDARY parameters

--- gas phase

     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,1=gas sat
         >>>> GAS PHASE
         >>>> PARAMETER : 1
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,2=gas rel per
         >>>> GAS PHASE
         >>>> PARAMETER : 2
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,3=gas visc
         >>>> GAS PHASE
         >>>> PARAMETER : 3
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,4=gas dens
         >>>> GAS PHASE
         >>>> PARAMETER : 4
         >>>> NO DATA
         <<<<
```

Figure 2.5.1. ITOUGH2 input file *vvi*.

```
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,5=gas enth
         >>>> GAS PHASE
         >>>> PARAMETER : 5
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,6=gas cap pres
         >>>> GAS PHASE
         >>>> PARAMETER : 6
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,7=Xwg
         >>>> GAS PHASE
         >>>> PARAMETER : 7
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 1,8=Xag
         >>>> GAS PHASE
         >>>> PARAMETER : 8
         >>>> NO DATA
         <<<<

--- liquid phase

     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,1=liq sat
         >>>> LIQUID PHASE
         >>>> PARAMETER : 1
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,2=liq rel per
         >>>> LIQUID PHASE
         >>>> PARAMETER : 2
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,3=liq visc
         >>>> LIQUID PHASE
         >>>> PARAMETER : 3
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,4=liq dens
         >>>> LIQUID PHASE
         >>>> PARAMETER : 4
         >>>> NO DATA
         <<<<
```

Figure 2.5.1. (cont.) ITOUGH2 input file *vvi*.

```
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,5=liq enth
         >>>> LIQUID PHASE
         >>>> PARAMETER : 5
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,6=liq cap pres
         >>>> LIQUID PHASE
         >>>> PARAMETER : 6
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,7=Xwl
         >>>> LIQUID PHASE
         >>>> PARAMETER : 7
         >>>> NO DATA
         <<<<
     >>> ELEMENT: ELM_1
         >>>> ANNOTATION: 2,8=Xal
         >>>> LIQUID PHASE
         >>>> PARAMETER : 8
         >>>> NO DATA
         <<<<
     <<<

--- the following block tests new observation type HEAT FLOW

  >> HEAT FLOW
     >>> CONNECTION:  ELM_1 ELM_2
         >>>> NO DATA
         <<<<
     <<<
  <<

> COMPUTATION
  >> OUTPUT
     >>> VERSION control statements
     >>> CHARACTERISTIC curves
     <<<

  >> OPTION
     >>> FORWARD
     <<<
  <<
<
```

Figure 2.5.1. (cont.) ITOUGH2 input file *vvi*.

Figure 2.5.2 shows an excerpt from the TOUGH2 output file. As a result of option MOP(5)=8, the secondary parameters as stored in TOUGH2 vector PAR are printed for gridblock "ELM 1", providing information about viscosity, specific enthalpy, and water mass fractions not available in the standard TOUGH2 output file. Saturation, relative permeability, capillary pressure, air mass fractions, and phase densities can be taken from the standard TOUGH2 output. Heat flow across interface "ELM 2 ELM 1" is -353.11 W.

Figure 2.5.3 shows an excerpt from the ITOUGH2 output file *vvi.out*. The column under header "COMPUTED" holds the selected observations extracted from TOUGH2 vector PAR and GLO for the specified gridblock and connection, respectively.

The values given in column "COMPUTED" of file *vvi.out* (Figure 2.5.3) and the corresponding output variables in the TOUGH2 output file (Figure 2.5.2) are identical, confirming the correct implementation of Requirement 5.